OFFICE OF NAVAL RESEARCH

CONTRACT N00014-95-1-0028

R&T Code 33e 1806

Dr. Richard S. Miller

Technical Report No. 91

SOME COMPUTATIONALLY-PREDICTED PROPERTIES
OF A GROUP OF PROPOSED ENERGETIC COMPOUNDS

by

Peter Politzer, Pat Lane and M. Edward Grice

Department of Chemistry
University of New Orleans
New Orleans, LA 70148

June 4, 1996

19960624 250

REPORT DOCUMENTATION PAGE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE June 4, 1996	3. REPORT TYPE AND DATES COVERED Technical

4. TITLE AND SUBTITLE
Some Computationally-Predicted Properties of a Group of Proposed Energetic Compounds

5. FUNDING NUMBERS
N00014-95-1-0028

Dr. Richard S. Miller

R&T Code 33e 1806

6. AUTHOR(S)
Peter Politzer, Pat Lane and M. Edward Grice

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

University of New Orleans
Department of Chemistry
New Orleans, Louisiana 70148

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research
Code 333
800 N. Quincy Street
Arlington, VA 22217

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release.
Unlimited distribution.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

We have carried out computational analyses and predictions of certain properties for a group of proposed energetic target compounds. The properties reported are: Heat of formation, 298 K, gaseous; heat of sublimation, 298 K; heat of formation, 298 K, solid; heat of fusion at melting point; heat of vaporization at boiling point; density, liquid; boiling point; impact sensitivity. Of the molecules considered, 1,3,5,7-tetranitro-2,4,6,8-tetraazacubane is particularly promising as a potential energetic compound.

14. SUBJECT TERMS
heat of formation, heat of sublimation, heat of fusion, heat of vaporization, liquid density, boiling point, impact sensitivity

15. NUMBER OF PAGES
6

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT Unlimited

We have carried out computational analyses and predictions of certain properties for a group of structures that were proposed by H. L. Ammon (University of Maryland) as potential energetic target compounds. The properties that will be reported, and the references describing the computational methods used, are as follows:

Heat of formation, 298 K, gaseous: ΔH_f (g), reference 1.

Heat of sublimation, 298 K: ΔH_{sub}, reference 2.

Heat of formation, 298 K, solid: ΔH_f (s)

$$\Delta H_f \text{ (s)} = \Delta H_f \text{ (g)} - \Delta H_{sub}$$

Heat of fusion at melting point: ΔH_{fus} (mp), reference 3.

Heat of vaporization at boiling point: ΔH_{vap} (bp), reference 4.

Density, liquid; reference 3.

Boiling point; reference 5.

Sensitivity: Estimates of impact sensitivity are given for four structures and shock sensitivity for two; the references will be cited individually. To put these values in perspective, the measured sensitivities of RDX on these scales are: impact sensitivity = h_{50} = 26 cm; shock sensitivity = 2.5 inches. We do not presently have a procedure for estimating the sensitivities of NF_2 derivatives.

Comments:

(1) We do not give predictions of solid densities, because this has already been done by H. L. Ammon.

(2) ΔH_{sub} (298 K) $\neq \Delta H_{fus}$ (mp) + ΔH_{vap} (bp) due to the differences in temperatures.

(3) We do not presently have a procedure for predicting melting points; this is in progress.

Recommendation:

We have suggested earlier, on the basis of computational studies, that the 1,3,5,7-tetranitro-2,4,6,8-tetraazacubane **5** merits particular consideration as a potential energetic compound [J. S. Murray, J. M. Seminario and P. Politzer, Struct. Chem. **2**, 153 (1991)]. Further support for this recommendation is provided by the present predictions for (a) ΔH_f (solid) in calories/gram, which is what is relevant for energetic performance, (b) sensitivity, and (c) solid state density (2.138 g/cm^3, as calculated by H. L. Ammon).

References:

1. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem., 16, 654 (1995).

2. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.

3. J. S. Murray, T. Brinck and P. Politzer, Chem. Phys. 204, 289 (1996).

4. J. S. Murray and P. Politzer, in Quantitative Treatments Of Solute/Solvent Interactions, P. Politzer and J. S. Murray, eds., Vol 1, Elsevier, Amsterdam, 1994, Chapter 8.

5. J. S. Murray, P. Lane, T. Brinck, K. Paulsen, M. E. Grice and P. Politzer, J. Phys. Chem. 97, 9369 (1993).

6. J. S. Murray, P. Lane and P. Politzer, Mol. Phys. 85, 1 (1995).

7. J. S. Murray and M. E. Grice, code PREDICTOR, U. S. Army Armament, Research, Development and Engineering Center, Dover, NJ.

8. P. Lane, unpublished work.

1
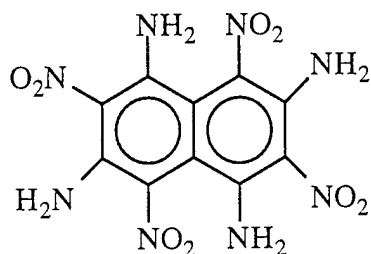
ΔH_f (g) = 17 kcal/mole

ΔH_f (s) = –24 kcal/mole = –65 cal/g

ΔH_{sub} (298 K) = 41 kcal/mole

ΔH_{fus} (mp) = 7 kcal/mole

ΔH_{vap} (bp) = 18 kcal/mole

Density (liquid) = 1.82 g/cm^3

Boiling pt. = 576 °C
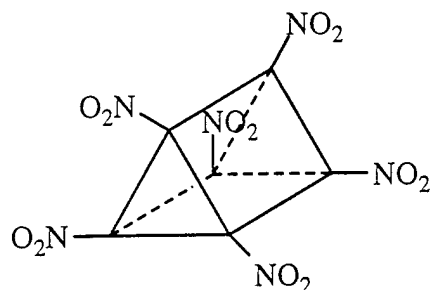
Impact sensitivity: h_{50} >> 320 cm (ref. 6)

2
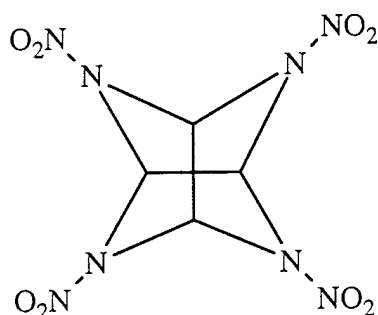
ΔH_f (g) = 114 kcal/mole

ΔH_f (s) = 84 kcal/mole = 288 cal/g

ΔH_{sub} (298 K) = 30 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 15 kcal/mole

Density (liquid) = 1.82 g/cm^3

Boiling pt. = 425 °C

Impact sensitivity: h_{50} = 42 cm (ref. 7)
                      h_{50} = 37 cm (ref. 8)

Shock sensitivity: 2.4 inches (ref. 7)

3
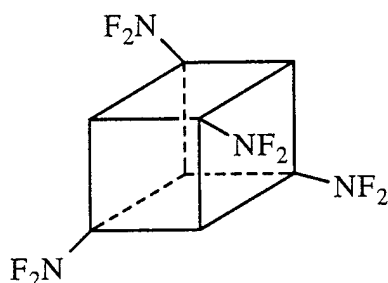
ΔH_f (g) = 73 kcal/mole

ΔH_f (s) = 43 kcal/mole = 141 cal/g

ΔH_{sub} (298 K) = 30 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 15 kcal/mole

Density (liquid) = 1.76 g/cm^3

Boiling pt. = 415 °C

4

ΔH_f (g) = 179 kcal/mole

ΔH_f (s) = 144 kcal/mole = 414 cal/g

ΔH_{sub} (298 K) = 35 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 16 kcal/mole

Density (liquid) = 1.89 g/cm^3

Boiling pt. = 487 °C

Impact sensitivity: h_{50} = 6 cm (ref. 7)

Shock sensitivity = 2.7 inches (ref. 7)

5
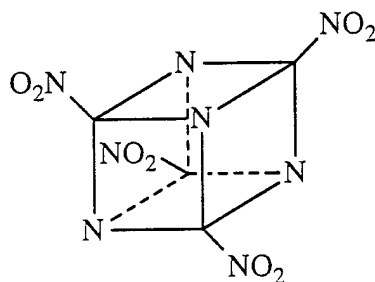
ΔH_f (g) = 216 kcal/mole

ΔH_f (s) = 189 kcal/mole = 656 cal/g

ΔH_{sub} (298 K) = 28 kcal/mole

ΔH_{fus} (mp) = 4 kcal/mole

ΔH_{vap} (bp) = 14 kcal/mole

Density (liquid) = 1.83 g/cm^3

Boiling pt. = 389 °C

Impact sensitivity: h_{50} < 160 cm (ref. 6)

6
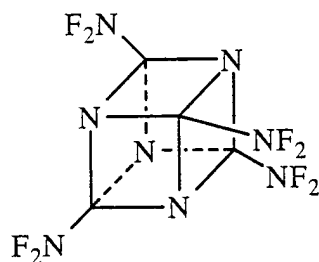
ΔH_f (g) = 141 kcal/mole

ΔH_f (s) = 114 kcal/mole = 365 cal/g

ΔH_{sub} (298 K) = 27 kcal/mole

ΔH_{fus} (mp) = 5 kcal/mole

ΔH_{vap} (bp) = 14 kcal/mole

Density (liquid) = 1.88 g/cm^3

Boiling pt. = 381 °C